2-PHENYL-9aH-BENZO[5,6]PYRIDO[1,2,3-c,d]AZAPENTALENE

N. S. Prostakov, A. T. Soldatenkov, and M. V. Bagdadi

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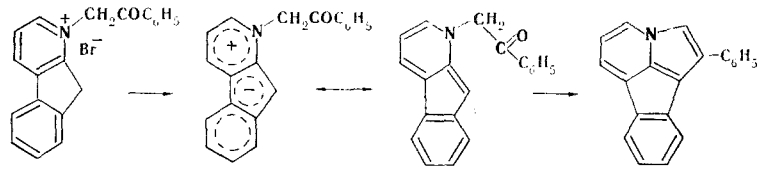
Condensed heterocyclic systems of the azadibenzopentalene type have been unknown up until now. Compounds of this type should evidently be classified as nonalternant π-electron systems — dibenzopentalene analogs [1] — under the condition of participation of the pair of electrons of the nitrogen atom of their indolizine fragment in conjugation.

We attempted to obtain the first representative of compounds of this series from 1-phenacyl-1-azafluorenium bromide (I) under the conditions of the Chichibabin reaction as applied to the synthesis of indenoindolizines from azafluorene salts [2], as well as from the pseudoazulene — 1H-1-phenacylindeno[2,1-b]pyridine (II) — formed under these conditions from salt I. Cyclization does not occur in either case, probably as a consequence of solvation in solution of the dipolar pseudoazulene II molecules.

2-Phenyl-9aH-benzo[5,6]pyrido[1,2,3-c,d]azapentalene (III) was obtained in 34% yield by heating pseudoazulene II *in vacuo* at 140°C and 20 mm for 4 h. It was isolated chromatographically in the form of dark-violet crystals with mp 132-134°C (from acetone). PMR spectrum (d_6-acetone): 7.04 (t, J = 6.5 Hz, 8-H), 7.65 (d, J = 6.5 Hz, 7-H), 7.75 (s, 1-H), and 8.31 ppm (d, J = 6.5 Hz, 9-H). UV spectrum, λ_{max}: 500 and 530 nm. The analytical and mass-spectral data confirm the structure of III. It may be assumed that the conversion of



I II III

pseudoazulene II to benzopyridoazapentalene III proceeds through a step involving intramolecular electrophilic attack by the carbonyl group of the phenacyl grouping on the C_9 position. This was confirmed by the fact that an analog of III with a p-nitrophenyl group attached to C_2 was obtained under the same conditions in 53% yield, whereas 1H-7-nitro-1-phenacylindeno[2,1-b]pyridine does not undergo cyclization even when it is heated for a considerably longer time.

LITERATURE CITED

1. K. Ingold, Theoretical Foundations of Organic Chemistry [Russian translation], Mir, Moscow (1973), p. 170.
2. N. S. Prostakov and O. B. Baktibaev, Khim. Geterotsikl. Soedin., No. 10, 1395 (1971).

Patrice Lumumba Peoples' Friendship University, Moscow 117923. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 5, pp. 705-706, May, 1982. Original article submitted September 5, 1981.

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